Ab Initio Simulations of the Photoemission of Hydrogenated Silicon Clusters

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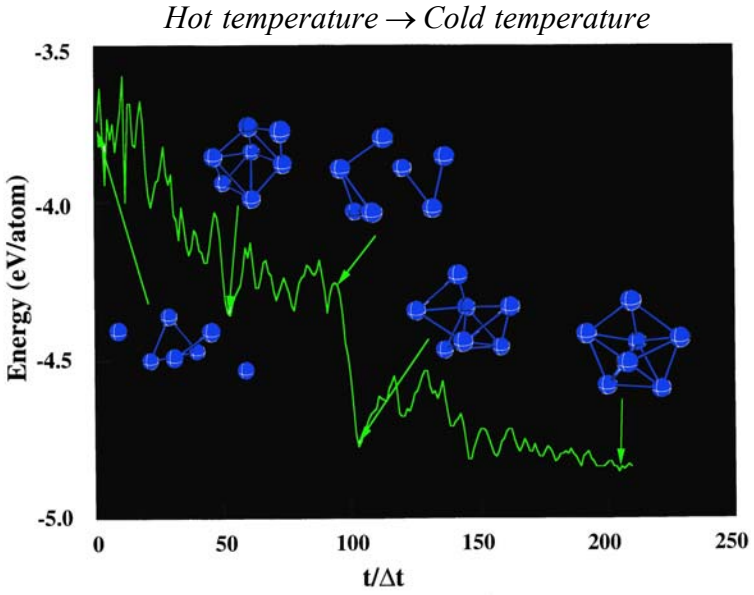
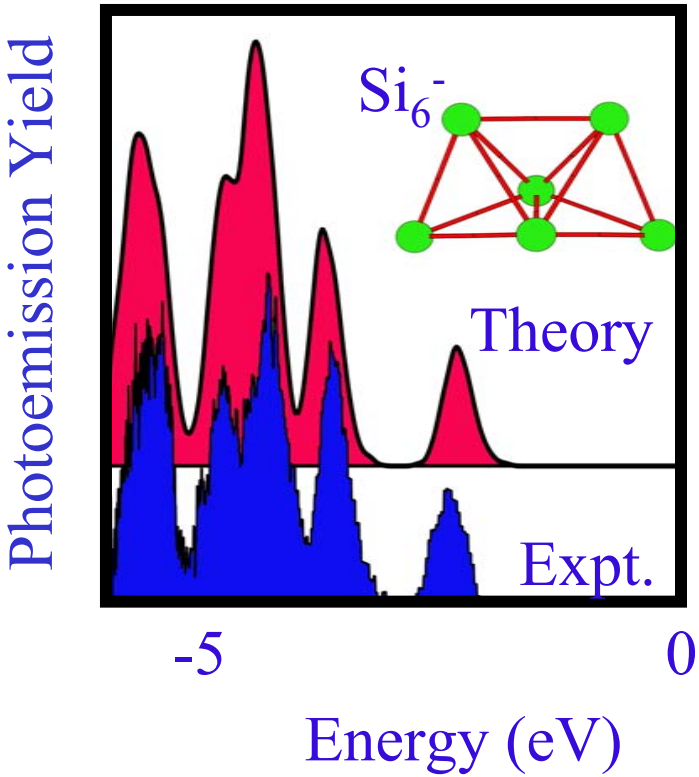
Clusters are isolated assemblages of atoms in metastable configurations. These systems are of great interest as they allow us to examine forms of matter that resemble neither isolated atoms nor solids. There are numerous unresolved issues about such systems. For example: What are the electronic and structural properties of clusters? How big does a cluster have to be to assume a crystal-like structure? These issues become more important as the size of electronic devices become smaller and smaller. As a first step in this process, we have worked with a group in Germany led by Gerd Ganteför. They have measured the photoemission spectra of hydrogenated silicon clusters. Our group has modeled the spectra of these clusters by using ab initio molecular dynamics, i.e., by calculating the quantum forces between atoms. In order to determine the structure of the clusters, we use simulated annealing. In this process, atoms at a high temperature are cooled until a cluster forms (top right figure). The resulting cluster is then placed in a heat bath characteristic of the experimental condition. The electronic energy distributions of the cluster is determined by averaging over ensembles of these clusters. The calculated photoemission spectra are in good agreement with experiment (an example is shown bottom right figure).

Nature: Materials 1, 49 (2002).





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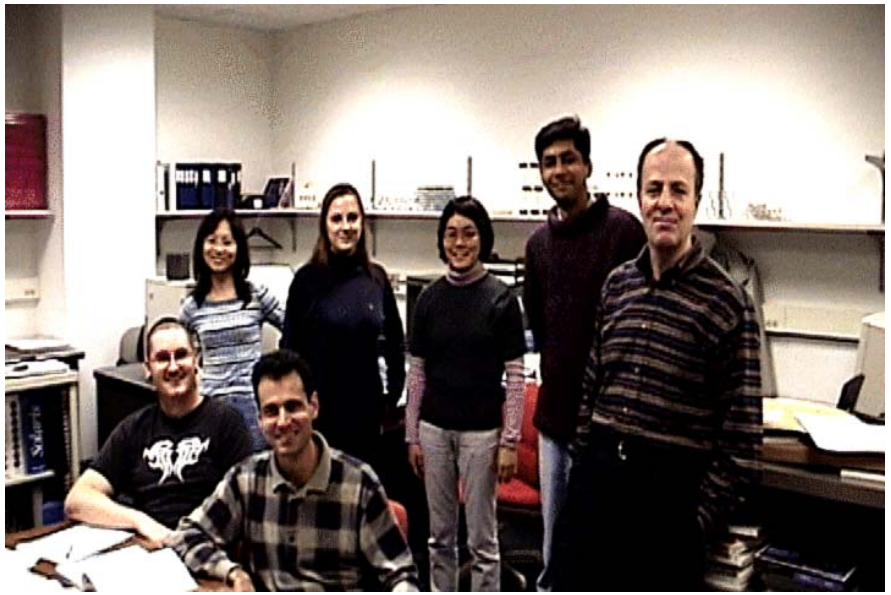
Educational:
5 grad students
3 post-docs.
Training centers on computational materials science, physics, chemical physics, scientific computation and computer science. Current research projects include magnetic semiconductors, semiconductor liquids, clusters, quantum dots and high performance, scalable algorithms for materials problems.

Outreach:
Web site for the distribution of computer codes and computational materials science. Open house in Department of Chemical Engineering and Materials Science. Computer simulation collaborations with high school science teachers.



Research group (left to right). Front row: Russ Burdick and Leeor Kronik. Back row: Shen Li, Claudia Troparevsky, Eunjung Ko, Manish Jain and Yousef Saad. (Some members not shown.)